Foundations of Computational Materials Modelling
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Introduction to Bravais lattices and constructing simple crystals with MATLAB

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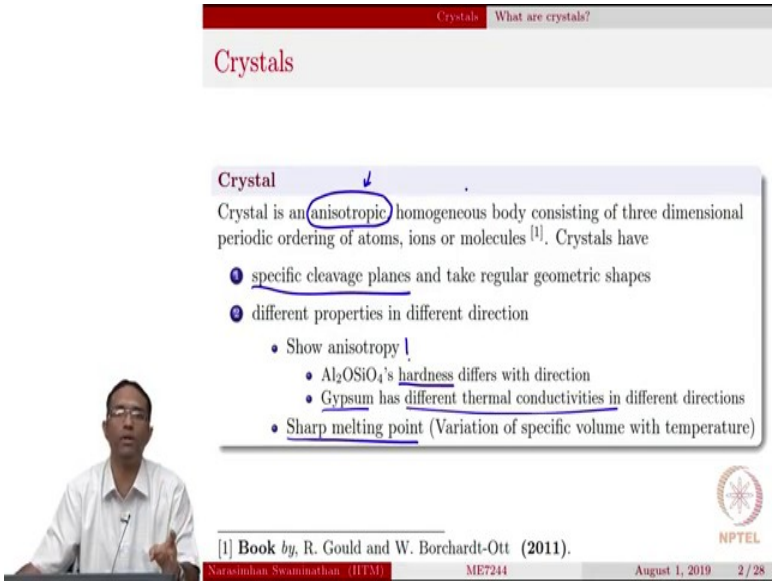

Welcome to this course on foundations of computation materials modeling. So last class we had a brief introduction as to what we will be studying in this course. Just to have a short recap of that, this course is divided in three modules. The first part will be dealing with constructing crystal structures on which you can perform some sort of analysis on the computer. The second part will essentially be statistical mechanics, where we will learn some foundations that is require for us to understand some elements of molecular dynamics simulations.

And the third part will deal with molecular dynamics simulations using labs. So the first part deals with constructing these crystals on the computer so that some analysis can be done. So in order to do that we need some fundamentals and we will start with the describing what exactly crystals are. So crystal is essentially something which is an anisotropic, which is homogeneous and processing some sort of three dimensional periodic ordering of atoms, ions or molecules.

It is important to understand that in general a single crystal is anisotropic which means it does not possess the same kind of properties in all the directions or it does not possess the same properties in all the directions. So these crystals turn out to be having specific planes and take regular geometric shapes. For example, if you take diamond crystal, then it will have a

specific cleavage, planes that will naturally appear when you are handling this particular material.

They have different properties in different directions, which essentially means show anisotropy. For instance, if you take Al_2OSiO_4, the hardness of this particular material happens to be different in different directions. So if you perform a scratch in one specific direction and then do the same thing in another different directions the forces that are required to perform the scratches on this particular material differs with direction. So that is what I mean by the word hardness here.

And then you can look at various other properties also. For instance, if you talk about gypsum, it has different thermal conductivities in different directions. So depending upon what direction the heat is traveling, it has a different resistance to heat flow. And then all crystals will show some sort of a sharp melting point that is associated when you are actually changing the face of the material.

So these are some of the properties that a crystal will generally possess but it is important for us to understand that they are generally anisotropic not isotropic. So a single crystal copper is an anisotropic material, it becomes isotopic only because of the fact that when you take a dog bones sample for performing a tensile test, you will generally measure only isotopic properties, although it is copper. And that is because various grains that are present in the copper material are oriented in random ways and all of these grains together give you a on an average anisotropic property.

But if you take each and every grain per se, they will have different mechanical properties, thermal properties also in different directions.

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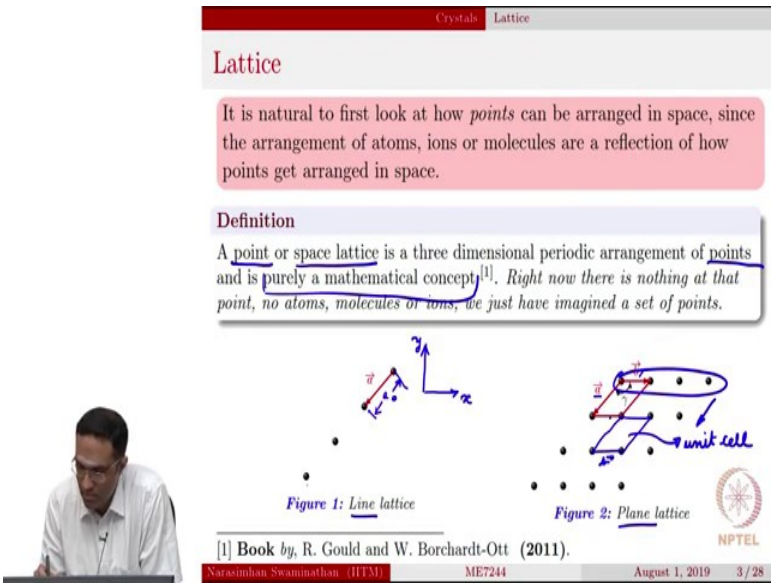

So before we start looking at how to construct crystals and understand some nomenclature related to crystallography which will help us construct complicated crystal structures, we start with the concept of a lattice. So lattice concept is associated with understanding how points can be arranged in three dimensional space. This is because you know when you are talking about arrangement of atoms or ions or molecules, they all are a reflection of how actually points are actually arranged in three dimensional space.

So a point or a space lattice is a three dimensional periodic arrangement of points. So when we say points here, at this point, we are only referring to a purely mathematical concept, which means that it is an imaginary point in space and there is nothing placed at that point So it is important for us to hold on to this idea that there are only imaginary points and no specific object that is being placed at that point or around that point.

So for example, you can have a set of points which are just forming a one dimensional lattice, so you can take this point and then repeat it with a certain repeat value, say say this, the distance is probably a_0, obviously, the direction in which you repeat it has to be given with respect to some coordinate system And it is repeated in three dimensional space and there is nothing in between these points and this is a lattice point that we are mentioning.

This is a one dimensional lattice or a line lattice, So to speak. We also can have space lattices. So in plane lattices you have these points repeating themselves in a certain pattern and they form a two dimensional array of lattice points. So you again repeat the lattice point in one direction and then repeat the entire thing in another direction. For example, in this case you

have first formed this lattice and then probably repeated it in the other direction going this way.

Consequently, you have two different lattice vectors that is associated with generating this lattice, the a vector and the b vector and there is naturally an included angle that occurs when you perform these, when you generate these space lattices. So this is the space lattice and as you all might be aware, something like this that is joining all these lattice points is called a unit cell and repeating that particular unit cell along these lattice vectors will essentially generate the entire plane lattice for you.

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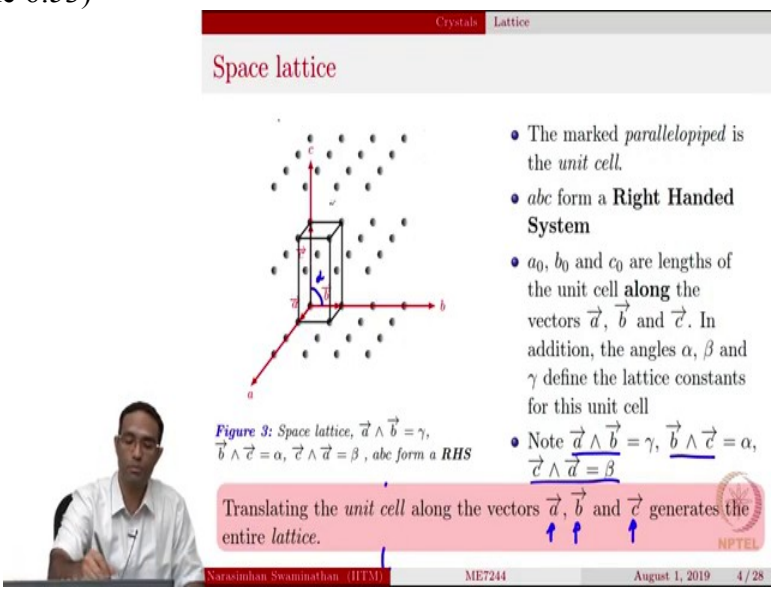

In a similar manner, we can look at what is referred to as space lattices. Space lattice is nothing but three dimensional periodic arrangement of lattice points. So in this simple figure, we have several lattice points, which are first being say repeated in the a direction and this entire line is then being repeated in the b direction to form this plane lattice and this entire plane lattice is then repeated in the c direction or you know, for clarity we could probably take this one and then say that this entire plane lattice is being repeated in the c direction to create a three dimensional space lattice,

This parallelopiped that is now naturally forming here could be a unit cell that is associated with this space lattice. And these vectors, a vector, b vector and c vector about which the repetition is actually taking place are called as lattice vectors and the dimensions of the unit cell, any parameter that is characterizing the unit cell, shape and size, say for example, this is

a_0, this value is b_0 and this value is c_0, together with included angles that may be related, characterize the lattice parameters

And it is a good question to ask as to how do we, what is the nomenclature or what is the convention that is followed in order to name these angles. So it is very simple. There is a very simple way to remember these things. So you have three angles that are generally used whenever we talk about the unit cell parameters or lattice parameters, alpha, beta and gamma. So alpha is the angle that is formed by the two vectors which is opposite to that of a. So a alpha can be related.

So this is alpha. Anything that is opposite to the b vector is basically beta and the angle that is opposite to the c vector is basically gamma. So this will be alpha and this would be beta and that is what is indicated in these lines. So angle between a and b is gamma angle, between b and c is alpha angle, between c and a is basically beta. And then again as we just looked at this plane lattice, repeating that particular unit cell in three dimensions along the lattice vectors, what is most important is you have to repeat these unit cells along the specific lattice vectors that is forming the unit cell itself will actually generate the entire space lattice for you.

So we are going to be using these simple concepts in order to generate complicated crystal structures in this course. It is a good idea to understand these things clearly.

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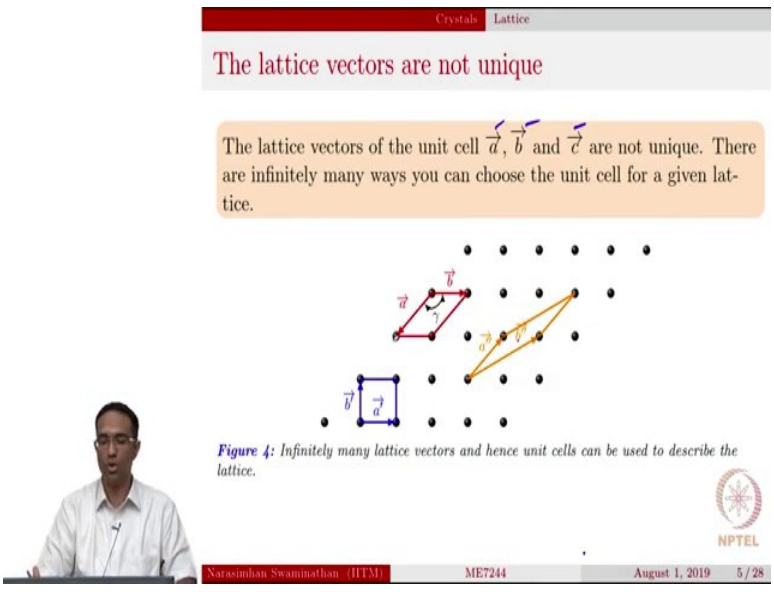

And then the final thing that is important when it comes to space lattices or plane lattices is to understand that the unit cell that you are essentially choosing is not unique. In order to

demonstrate that, let us look at this plane lattice. So you have an arrangement of lattice points in this direction. This has been repeated in some other direction, to result in the formation of the space lattice. Now, we might as well choose this very convenient looking, rectangular unit cell formed by a prime and b prime and repeat this entire thing in three dimensions.

So one of the most important things we need to understand is that this space lattice is repeating itself in two directions. It is going to infinite lengths in both, the x direction as well as in the y direction. We have drawn only some portion of it, but when I say lattice, it means it is extending to infinity in both directions.

So consequently when you want to generate this infinite lattice, you may choose a small unit cell which looks simple like that what is formed by a prime and b prime and you may repeat this in X and the Y, not in the in the along the a prime and b prime vectors in order to generate this lattice or you may also choose this complicated looking unit cell which is comprised now of vectors a double prime and b double prime, forming this slightly more complicated, weirdly shaped the unit cell.

And this also may now be repeated along a double prime to generate another unit cell here. So you may just take this one and move it along a double prime and b double prime in order to generate other unit cells. So this is another unit cell, this is another thing that is formed by repeating this in both the directions or you may also choose something like this and the idea is you may choose to translate it along the b vector and the a vector.

So what is important for us to understand is that you could either choose a simple unit cell or you could choose more complicated unit cells and the total number of unit cells that you can actually develop from this set of lattice points is infinity. So basically, there is no unique way by which you can actually choose either the lattice vectors or the unit cell in order to generate the entire space lattice or the plane lattice.

So these unit cells are generally chosen based on convenience and other considerations, such as the kind of symmetry that the unit cell has and the kind of symmetry that is present in the underlying lattice that you are trying to generate. So we will study those things as time goes on, but it is important for us to understand that the lattice vectors and the unit cell consequently are not a unique choice

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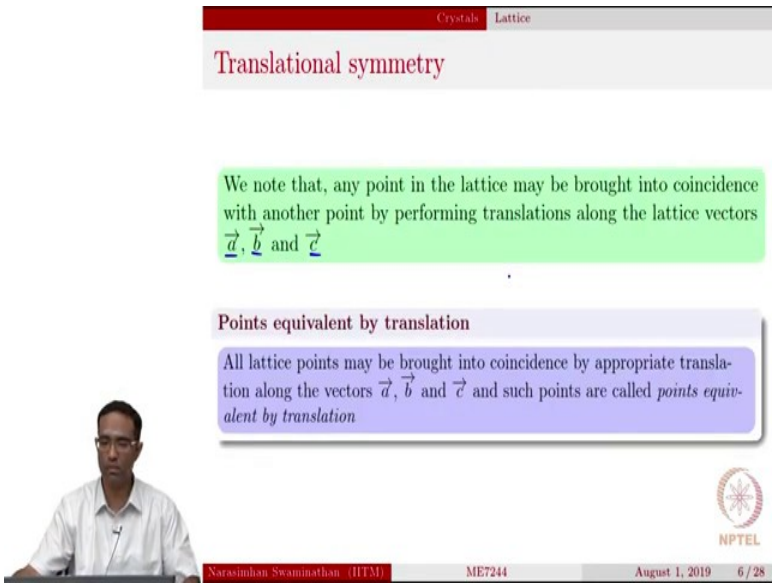

So any point in the lattice maybe brought into coincidence with itself with another point by performing translations along the A, B and C directions. So this must be quite clear. So you are able to bring a lattice into coinciding this lattice point with another point by moving along the lattice vectors. So these points are all points which are equivalent by translation.

So there is really no big difference for a being that is being present in this lattice point, or in this lattice point, everything is the same. Like I mentioned, this is easy to imagine if you think of it for a second and accept that this is actually a two dimensional infinite plane of lattice parts. So there is no big difference between this point and this point, they are all equivalent by translation.

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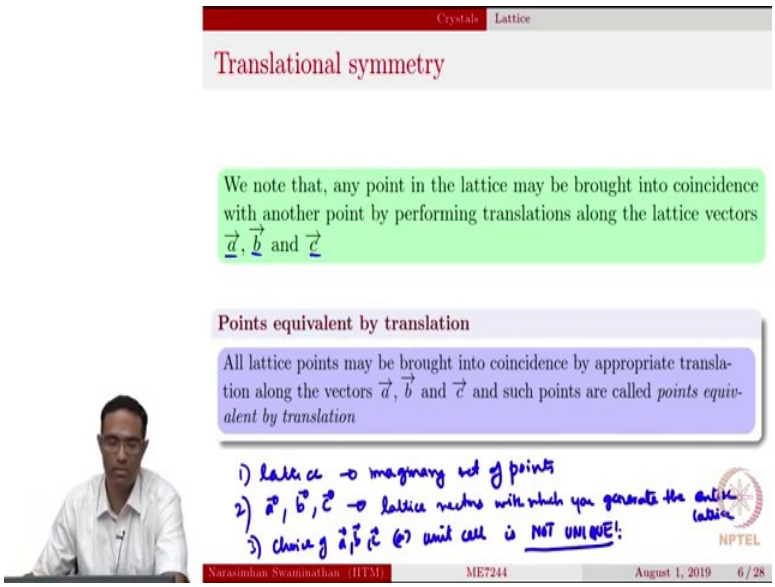

So with that, we have introduced what is referred to as a lattice. So in summary, we need to remember that when we talk only about a lattice, it is only imaginary set of points. The second point is - a vector, b vector, c vector or lattice vectors with which you generate the entire lattice. The choice a vector, b vector, c vector or the unit cell is not unique

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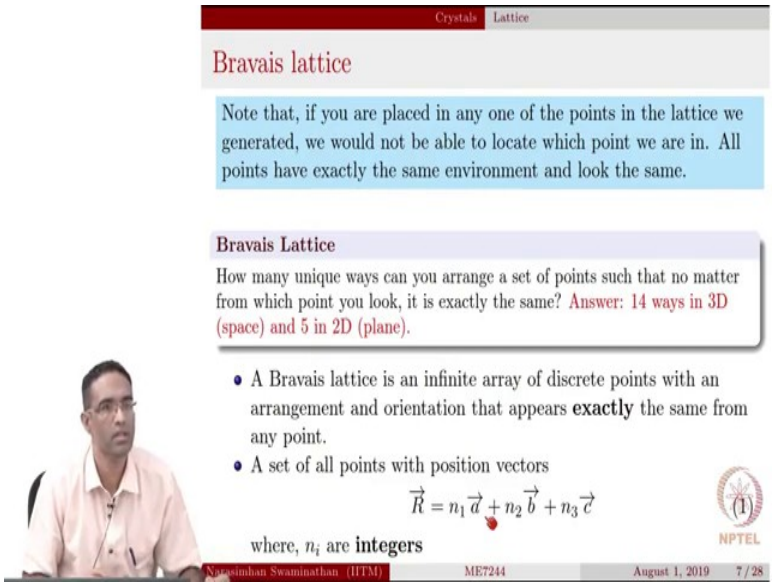

Then we come into the subject of Bravais lattice. So Bravais lattice so just like what I mentioned a couple of minutes back, if a beam, some beam is actually sitting on this point, it will not know whether it is sitting on this point or this point, because since the lattice is extending to infinity, it will not be able to make out the difference between this lattice point and this lattice point because the environment around this point is essentially the same whether it is sitting here or sitting here.

Such lattices which look exactly the same from any lattice point are referred to as Bravais lattices they are referred to as Bravais lattices. So consequently, using Bravais lattices to construct crystal structure is extremely useful. So the next question that we ask now is how many unique ways can we actually arrange a set of points in 3d space such that no matter from which point you look, it always appear the same.

So the answer to that question is 14 ways. In three dimensional space, you can arrange a set of points in three dimensional space in such a way that if you sit on any one point, it looks exactly the same always, is about 14 ways and in two dimension it happens to be 5 different ways or they are called us plane Bravais lattices and then this is a mathematical manner in which you can talk about this Bravais lattices.

If you want to represent this actually mathematically, this is the way to do it. So if you have a bunch of vectors, A vector, if you have a bunch of vectors A, B and C, and if you have different sets of integer n1, n2 and n3, it is possible for you to obtain the positions of the lattice vector using this expression right here, So this is what we are going to be using several times at least in the first part of this course in order to generate crystal structures as well, the same idea.

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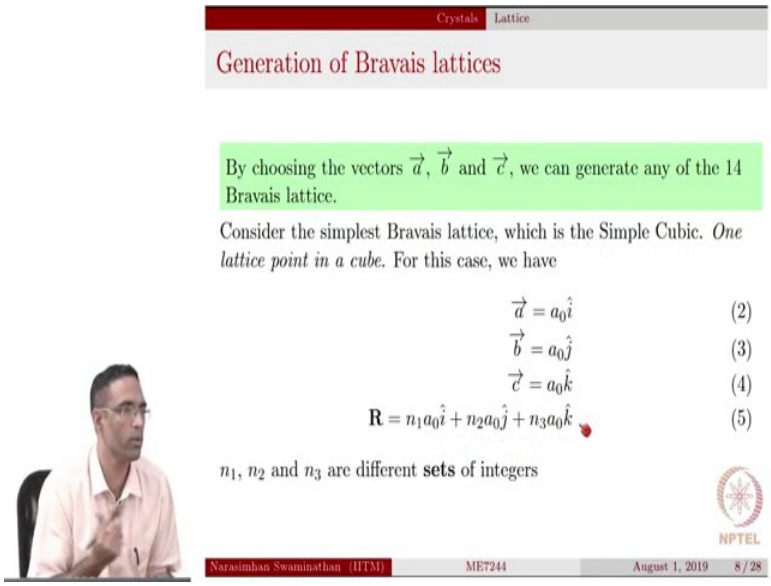

Let us take for example, the generation of a simple cubic lattice, which is a Bravais lattice. So if you take the Bravais lattice which is simple cubic, simple cubic in the sense, there is one lattice point inside the cube. There are, you must have studied in your basic material science that you have one, at every corner of the cube you have one lattice point, but that corner is being shared by 8 other cubes. So consequently you have 1 by 8 and 8 which gives you 1 lattice point per cube.

So but if you want to generate this using a computer program, So you choose your a vector as a_0 times I hat, b vector as a_0 times J had and c vector also as a_0 times k hat and any lattice point in the simple cubic structure is simply n1 a_0 i plus n2 a_0 j into n3 a_0 k. n1, n2, n3 are different sets of integers.

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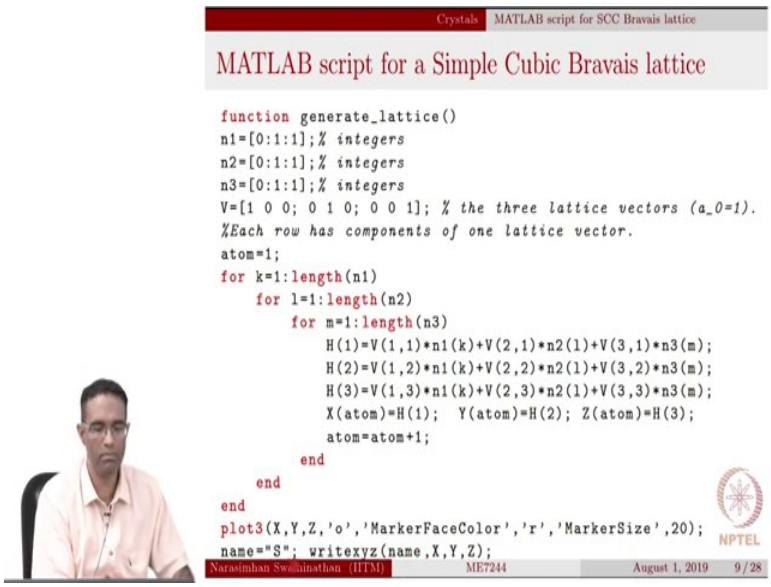

So without wasting too much time, I would like to introduce you to the actual MATLAB program that will actually generate this lattice. So I am sure you some of you at least might be familiar with MATLAB and if you are not, you can learn it very easily. So this is a MATLAB script for generating a simple cubic Bravais lattice. So this is, the first line is basically the function definition.

And you have three sets of integers each running from 0 to 1. So consequently, what will be generated out of this is just one unit cell of simple cubic lattice. V 100, 010, 001 are the three lattice vectors with a_0 being 1, so I have just chosen the lattice constant to be 1. For convenience, you can have anything there. Atom equal to 1 is just a counter and then there are three counters which run over the length of these vectors.

So you can modify the total number of unit cells that you want to create in the y direction and the z direction by just changing this one to some other number and this, the other one to some other number and so on and so forth. So each one the, first line, the second line and the third line basically capture the x coordinate the y coordinate and the z coordinate of each and every lattice point.

And this atom is just a counter. Consequently, we want to print the complete unit cell that we have generated. So the last command, plot 3 x y z, which will be a column vector of Xs, column vector of Ys and Zs will be used to actually print out the lattice, the simple cubic lattice. Now, whenever you are working with computational materials modelling, you do not use MATLAB to visualize these lattice structures.

There are several codes, programs which can read in files, read in coordinate files in different forms and show you the crystal structure. So usually that is very convenient. One such file format that is read by several codes is called as the XYZ format, which is one of the simplest format and there is a small function which I am calling here, which will actually take us a character called name, name is equal to s and it will take the corresponding x coordinates, y coordinates and z coordinates and it is going to give you the, it is going to write it out, write out the XYZ file for this simple cubic structure.

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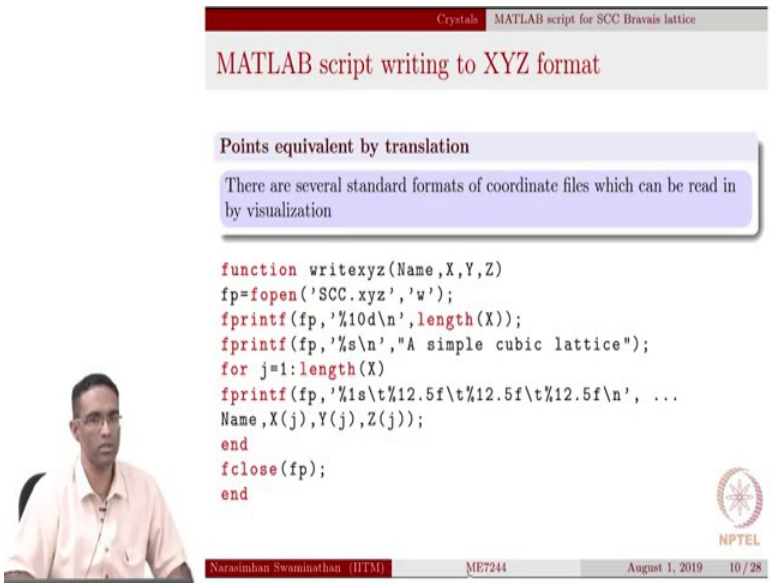

So this is the corresponding code which talks about this XYZ file.

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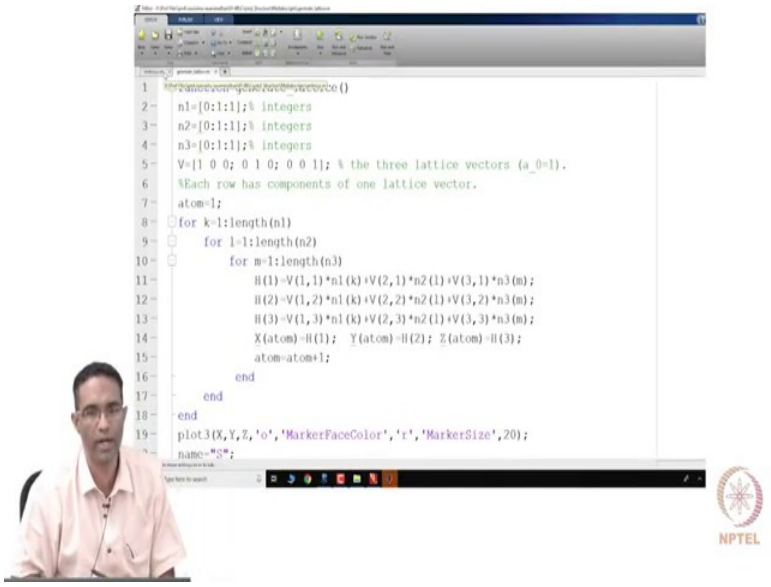

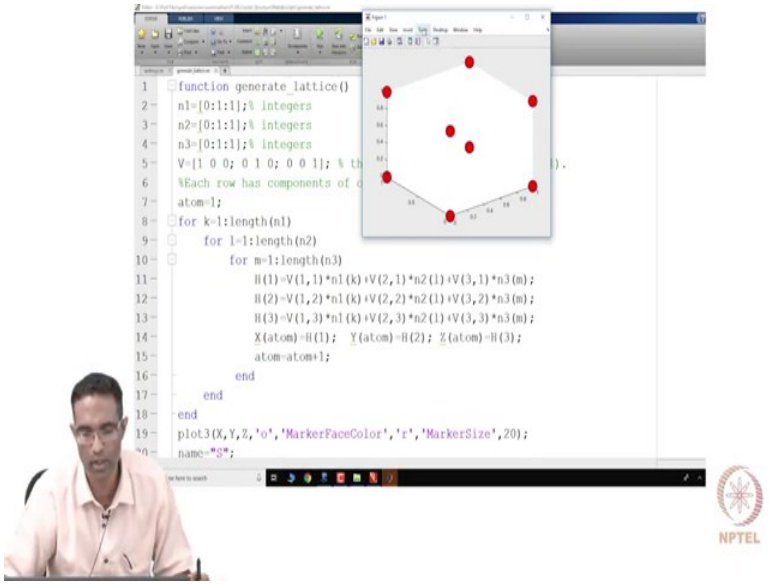

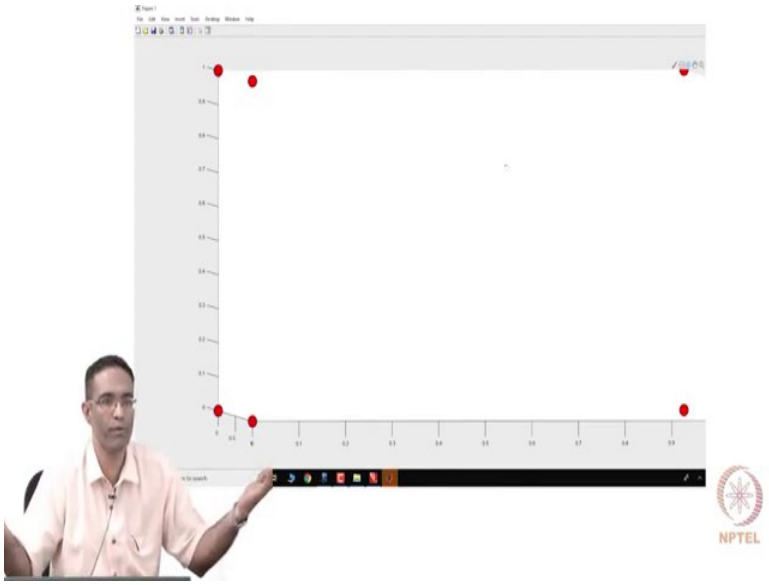

So I would like to show you the MATLAB script and what happens when it runs. So this is the Generate lead is exactly the same file that we talked about, so if you run it, you get a simple cubic lattice and you can actually rotate it and see, it is precisely that, it is precisely that. We are going to use this for our learning purposes, we do not professionally when we are doing research, this is not the kind of visualization we use.

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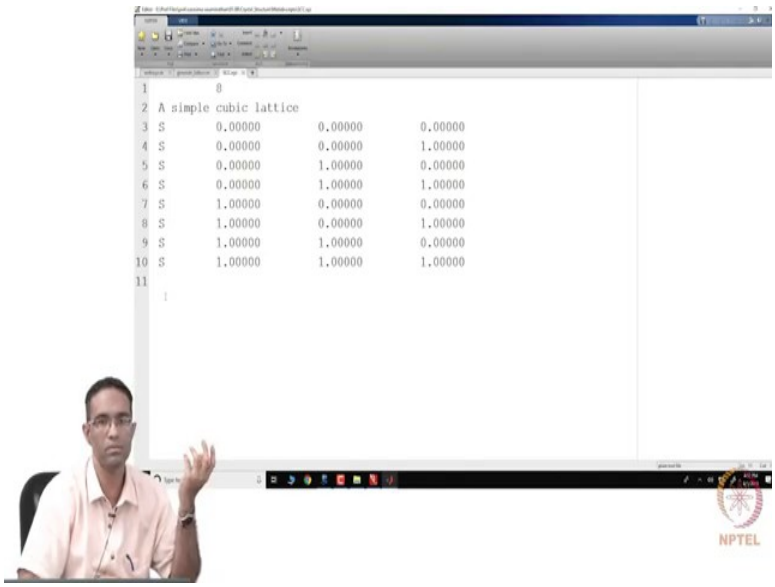

But it is possible for us to write out the XYZ file and take a look at. This is how the XYZ format looks. So in the first line, you have the total number of atoms that you are printing out. The total number of atoms in the unit cell is however, only one but when you want to visualize the unit cells with all the spheres, you want to print the coordinates out, so the total number of atoms is 8 and the second line is basically some sort of a string, which is used to tell you something about the crystal structure.

The first column is a symbol that is used to identify what type of atom it is. And the second, third and the fourth columns are basically the X, Y, Z coordinates. So this is what this programme does.

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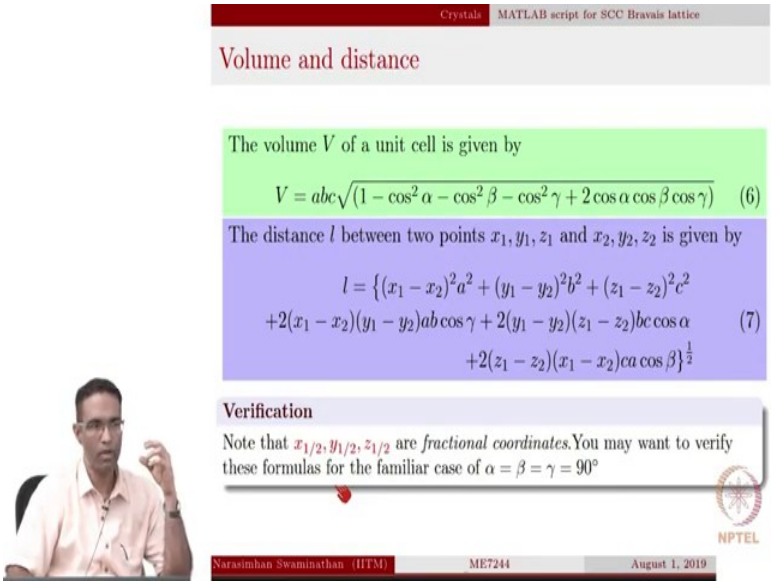

Now, off and on not all not all the unit cells that we deal with are cubic. You will encounter triclinic or monoclinic unit cells as well. So when you have a cubic structure, calculation of the volume or the distances between the points is pretty simple. However, when you have other non cubic structures, calculation of the volume and the calculation of the distances between points can be a little bit cumbersome, but if you do some vector algebra you can understand or you can convince yourself that the expression for calculating the volume is given by the expression number 6 here and the distances between two points, x1, y1, z1; x2, y2, z2 are given by the formula seven.

Here x1, y1, z1; x2, y2, z2 are basically the fractional coordinates between those two points. They are not the actual Cartesian coordinates. So it is very easy to verify that the first expression six is straightforward if you substitute alpha equal to 90, beta equal to 90 and gamma equal to 90, you talk about a orthogonal unit cell and the product of ABC is basically going to be your volume.

Now that is not the case if you have non cubic structures. So that is why I have just given this expression here, but it is not very hard for you to prove this yourself.

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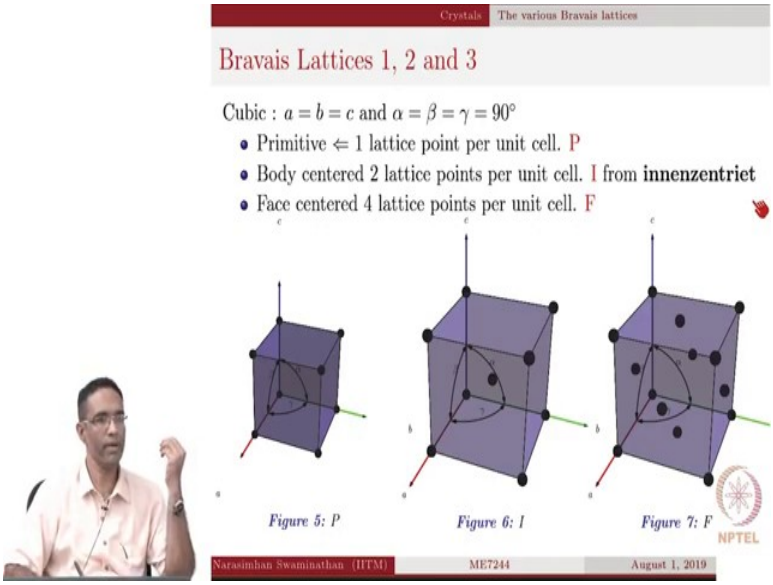

Now, let us start looking at the various Bravais lattices.

Professor- Student Begins

Professor: How many Bravais lattices are there? There are…

Student: 14.

Professor: What is that? 14 Bravais lattices are there.

Professor- Student conversation ends.

Now, these are extremely important because all of our crystal structures are based off these 14 Bravais lattices. So the first Bravais lattice as you know, Bravais lattice 1, 2 and 3 as they call it, they all will have A, B, C equal being equal and the angles between them are 90 degrees. In these Bravais lattices you have three different types- one is called primitive. We will come to the definition of primitive in just a bit.

The other one is called body centered, where you have two lattice points per unit cell and the third one is basically the face centered where you have four lattice points per unit cell. And there is a representation that is generally used when we talk about this Bravais lattice. P is for primitive, I is for body centered and F is for face centered. Remember, these symbols are going to be used again when we talk about symmetry.

So this P, this I and this F are representing primitive, body centered and face centered Bravais lattices.

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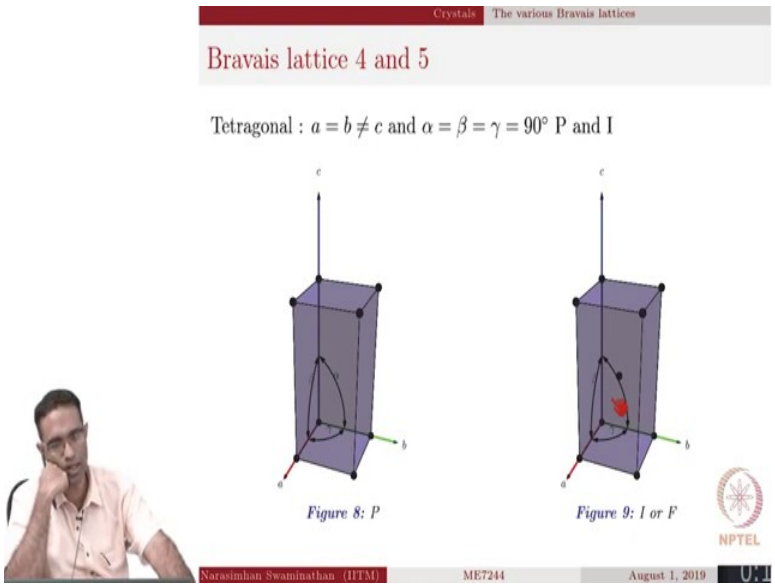

Lattices 4 and 5 have slightly lower symmetry, they are tetragonal, So A is equal to B so A and B are equal, C is not equal to A and B, and the angles between them are of course, 90 degrees and in this particular type of Bravais lattice you can either have a primitive or you can have a body centered lattice. The question now is why is there no both I and F in a tetragonal lattice. This is a tetragonal lattice, why is there no face centered tetragonal lattice?

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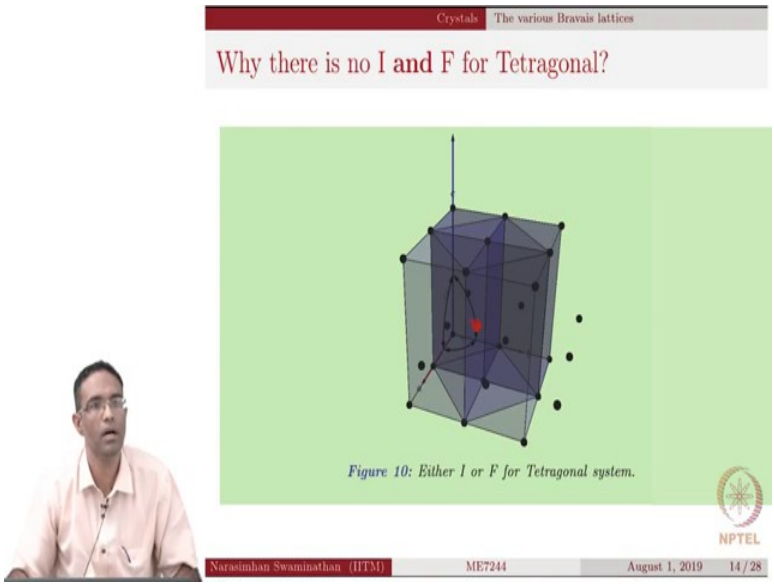

So the answer for that is if you take a look at, this is this particular figure here shows you the tetragonal lattice and you have one body centered here and a body centered atom for each of these. So this is actually the tetragonal lattice right here, and you have one body centered

atom here. Similarly for the next one you have one here, here and here. These are the body centers.

However, if you actually really look at it carefully and take a look at it, so you will once again be generating only a tetragonal face if you look at this, if you look at this tetragonal system that is drawn, you will find that the same atoms are forming the first centered tetragonal. So from a body centered tetragonal, we are able to regenerate the face centred tetragonal. So there is no point in counting them twice because they are basically the same lattice.

Consequently, you either talk about a body centered tetragonal or a face tetragonal the convention is to talk about the body centered tetragonal as the Bravais lattice

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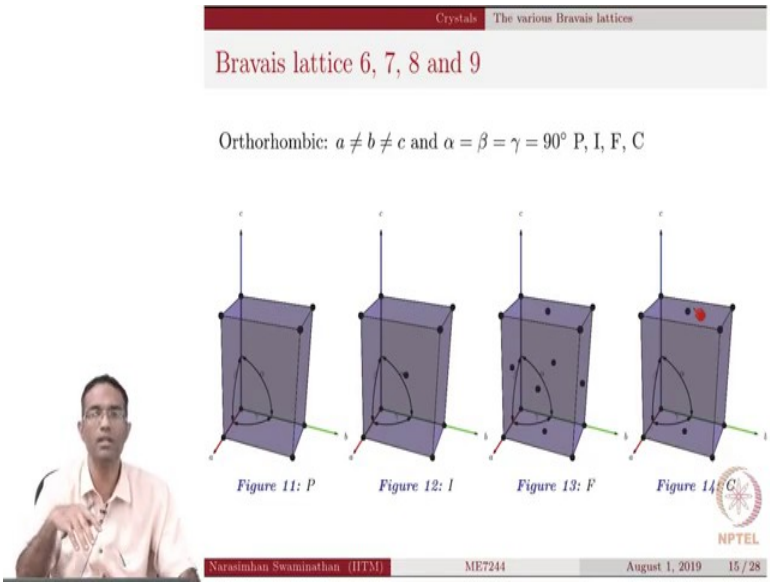

In this manner, if you actually looked at other things that are not listed here, you can convince yourself that they all turn out to be one of these 14 somehow, and we have some convention so that we understand when we talk about crystal structures, what we are, to stick to one particular convention we talk about one type of Bravais lattice for one particular system. So next one is the orthorhombic Bravais lattice.

In this you can have primitive, I, F and something called as C. So you have a centered latest. So at least at you will have at opposite phases you will have one lattice point that is going to be 6, 7, 8 and 9. So you have like 4 different versions of the orthorhombic Bravais lattice.

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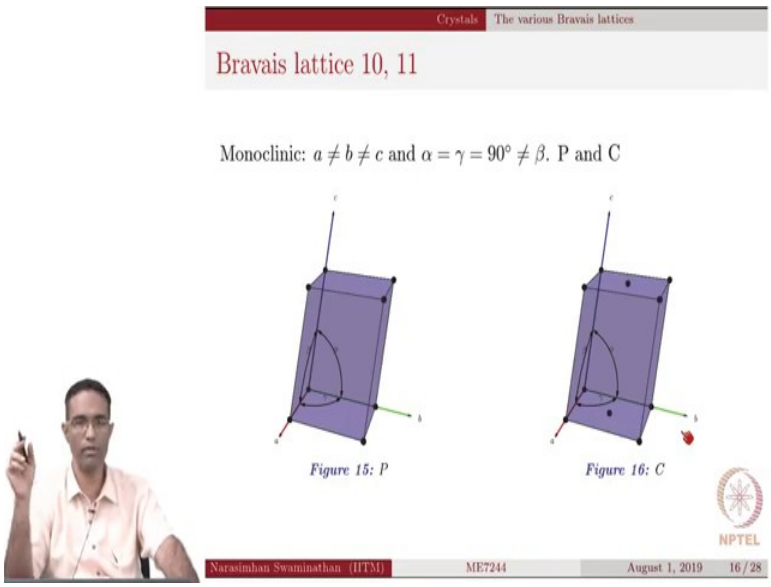

Then you have the monoclinic lattices where you have a none of them none of the sides are equal, but you will have one lattice vector being perpendicular to the other two, So one of the angles will not be equal to 90 degrees, the beta is not equal to 90 degrees and in this what is possible is P and C.

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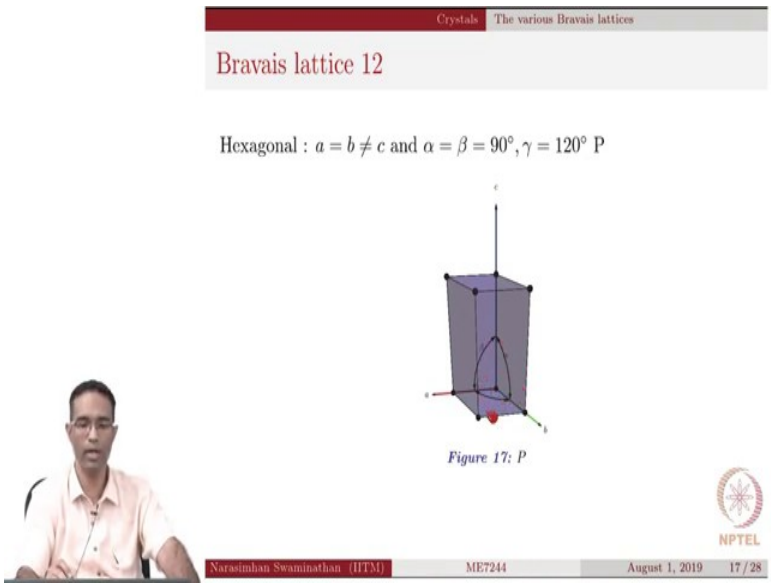

The 12th one is basically hexagonal. So there is going to be an angle gamma of 120 degrees, whereas the angle beta and alpha are both 90 degrees. In this the only thing that is possible is primitive. Anything else you do, it becomes one of the others.

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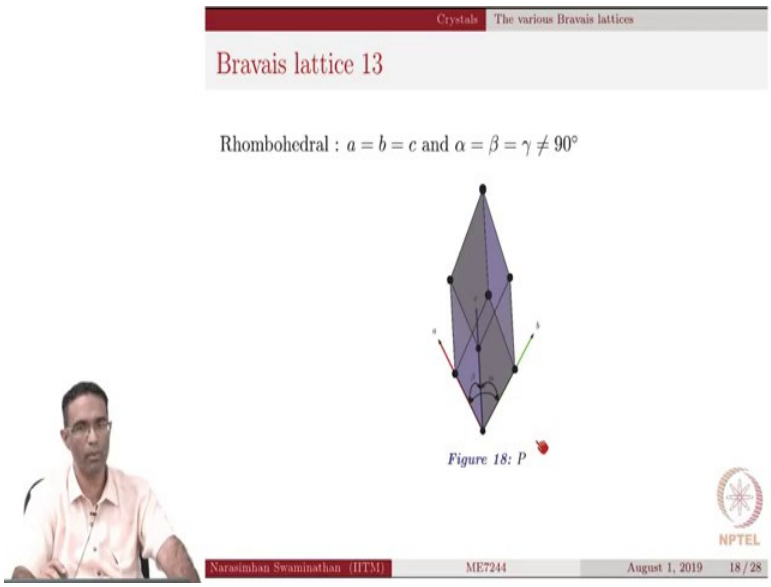

13th one is the rhombohedral, where you have A equal to B equal to C, and the included angle, alpha equal to beta equal to gamma. However, none of them are 90 degrees. The last one is basically the triclinic lattice where none of the sides are equal, and none of the angles are basically equal.

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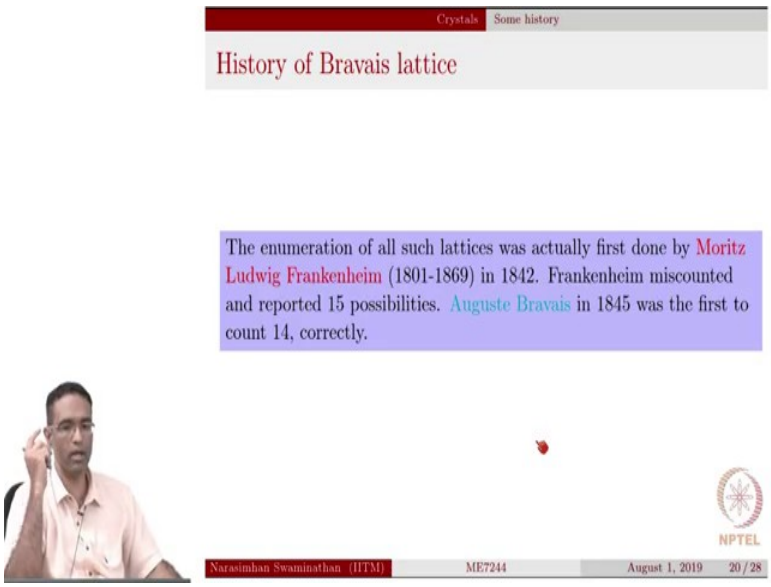

So these are the various Bravais lattices. There are 14 Bravais lattices. One of the interesting things that we see about Bravais lattices is its history. So the enumeration of all these lattices were actually done by someone called Moritz Ludwig Frankenheim in the year 1842. He

came up with actually 15 different Bravais lattices. He counted, he only did the major work, He came up with the 15 ones.

He counted one of them two times and then Bravais came in, Auguste Bravais came in in 1845 and he has corrected this 15 to 14. But you do not call them Frankenheim lattices, you still call them Bravais lattices. So that is an interesting history that comes out when you are studying these Bravais lattices.

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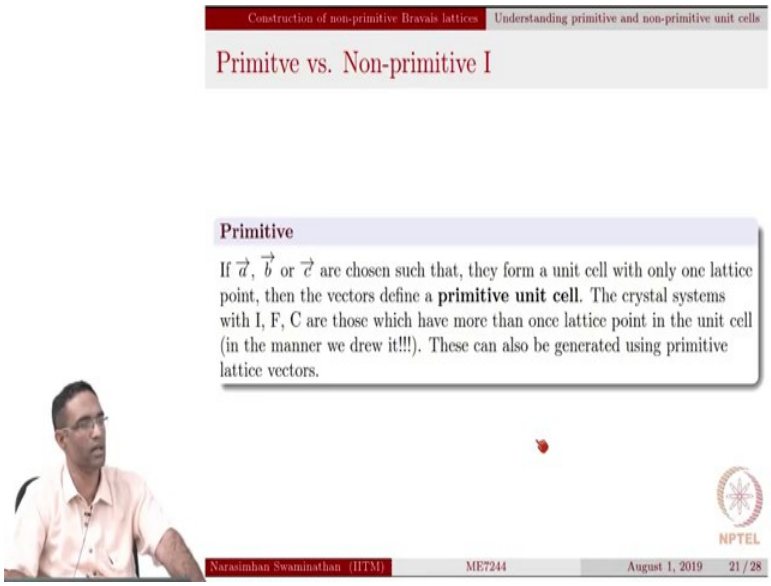

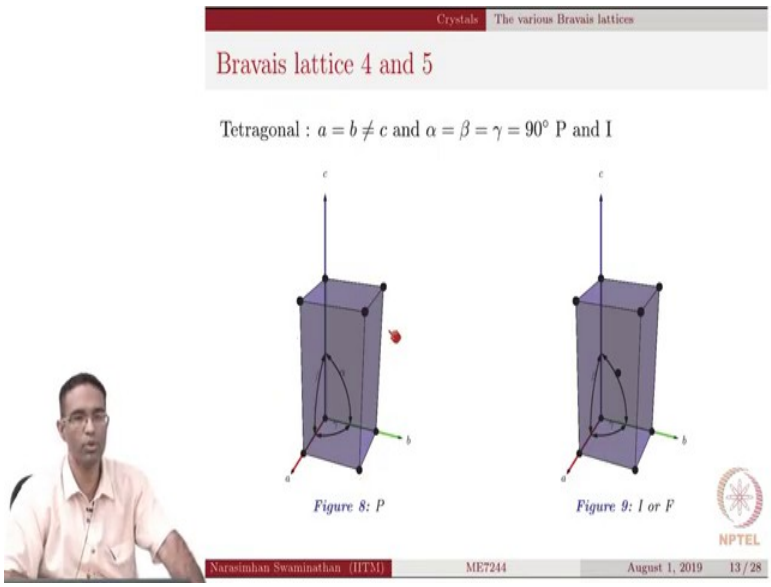

Now, one of the things that we now get into is the definition of a primitive lattice 2. So you have been seeing these Bravais lattices and several times you saw a P, You saw P several times. What was unique about that P? What was unique about that unit cell?

Professor- Student conversation begins.

Professor: What is that?

Student: You have atoms only at the corners.

Professor: You have atoms only at the corners.

Professor- Student conversation ends.

What that means is, you have only one lattice point per unit cell. So the definition of a primitive lattice is that you have only one lattice point per unit cell, all other lattices, the centered lattices, the face center lattices or the body centered lattices have more than one lattice per unit cell

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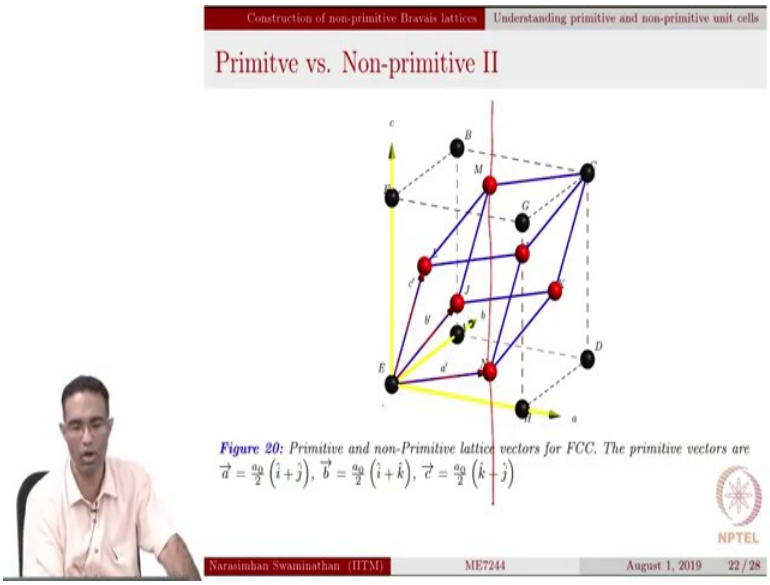

The question now arises, is it possible for us to construct or have primitive unit cells for all the Bravais lattices that we talked about? The answer is yes, So I will show you an example with FCC structures. So FCC, so this is an FCC structure In general how do you generate an FCC structure? You have A, you have your B lattice vector and your C lattice vector and you have one lattice point at all the corners and then these red points right here, are the face

centers and you have FCC lattice and that contains how many points how many lattice points per unit cell?

Student: 4.

4 lattice points per unit cell. Now, you look at the other unit cell that is drawn here in the blue color. So this point C is joined to the C dash, this I this N and then you have all these atoms and then these lines have joined and you see that, if you have just that as a unit cell, the total number of lattice points in that unit cell is only one. That can also be used as a unit cell, you can construct it and repeat it in three directions and generate your FCC lattice. It is still FCC,

The problem is your A is, the lattice vectors, a prime, b prime and c prime are not orthogonal. They have some weird included angle between them. However, your A, B and C that you used previously are all orthogonal, they are equal in length. And last but not the least, if you drew it using the non-primitive lattices, you are able to maintain the symmetry of the underlying lattice.

That means, if you rotate say for example, if you rotate this structure about a line suppose, you rotated the structure about this line by 90 degrees, the crystal structure would exactly coincide with itself, so this structure possesses some sort of symmetry. However, that is not apparent if you use the other unit cell. So in order to preserve the underlying symmetry of the lattice, we choose unit cells which are convenient.

Because once you know the symmetry of the underlying crystal structure from the unit cell itself then the kind of symmetry that is demonstrated by or the kind of symmetry shown by various properties of these materials also become apparent, so there is a reason why you want to choose these unit cells extremely carefully, But then it will become obvious as we go as to what unit cell must be chosen for what lattice based on the symmetry underlying the lattice.

So the primitive and non-primitive lattice vectors, so for FCC, the primitive lattice vectors are obviously these a_0 by 2 i plus jb, a_0 by 2 i plus K and a_0 by 2 k plus. However, the non-primitive lattice vectors is just ai, sorry this would be a_0 I, a_0 j and a_0 k,

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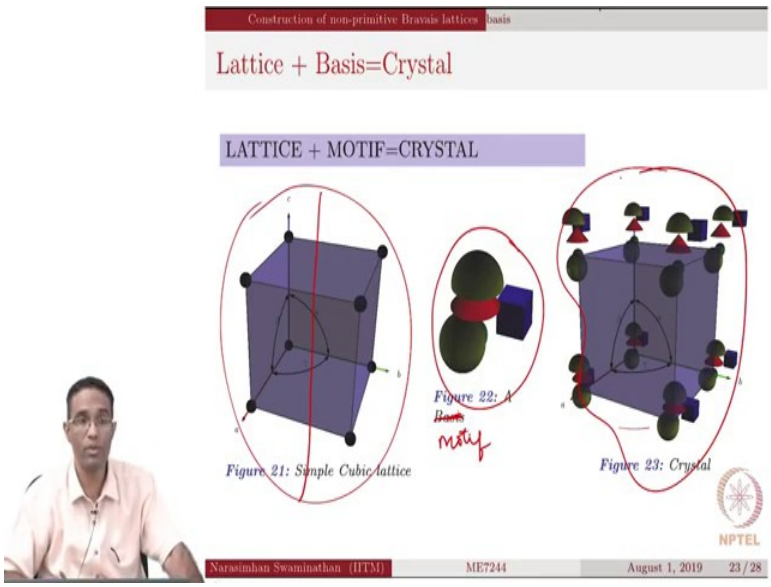

Now, we talked about lattice. What did I tell you about lattices? Lattice is nothing but a collection of imaginary points in space.

At this point, we have not yet put something. You know, we do not have an atom or an ion yet. It is just an imaginary mathematical construct. Now, at each point, if you start putting some motif, some molecule, then that basically becomes a crystal that is of interest to us. So this is a simple cubic lattice, it is extending to infinity in all the directions and this is some arbitrary motif, so this should be motif.

And at each point I am putting that motif. What you should observe is, this lattice which is a collection of these points alone had some symmetry associated with it. For example, it had a 4 fold symmetry about this point. But the second I put this motif at these points, some symmetry get lost, get lost, but the property of the crystal is actually going to depend on how these motif are basically arranged around the lattice points or at the lattice points, so to speak.

That is the reason why we need to start looking at these symmetry associated with these crystal structures. Do you have any questions at this point?

Professor-student conversation begins

Professor: Yes?

Student: Is there any difference between the points motif and basis

Professor: Yes. I will say yes, motif is probably the molecule that you use to put at every lattice point and basis is something slightly different which we will come to in a couple of slides. Sometimes they are used interchangeably also but I want to keep a clear distinction. Motif is this molecule that we will place and basis are points that we will choose so as to construct a crystal structure based on non-primitive lattice vectors

Student: So if instead of a molecule, I put items or items, they will also be called as motif.

Professor: You can call them as motif, yes, no problem. As long as we understand what it means is not a problem.

Professor-student conversation ends.

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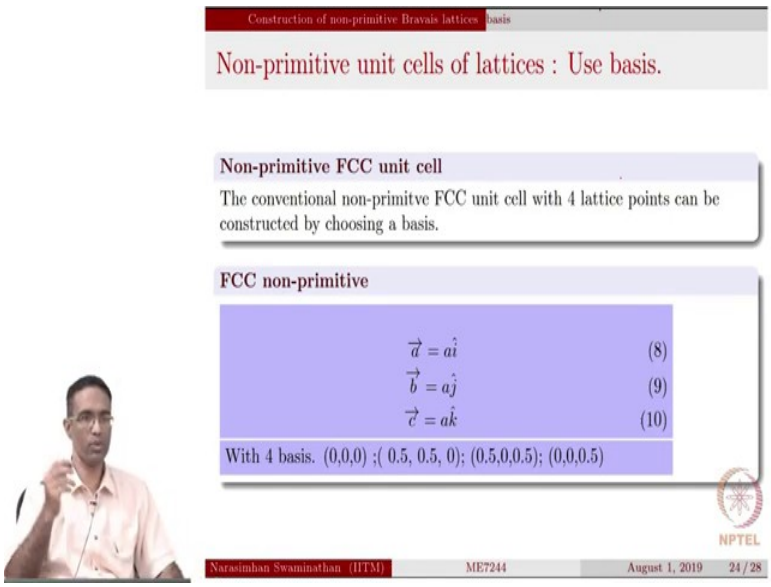

So actually trying to answer his question. So his question was is there a difference between basis and a motif. They are used interchangeably. However, in this lecture I would like to call motif as something that is placed around the lattice points, a molecule or the atom and basis as something that I will choose in order to construct lattice structures out of non-primitive basis vectors or lattice vectors, basis or lattice vectors.

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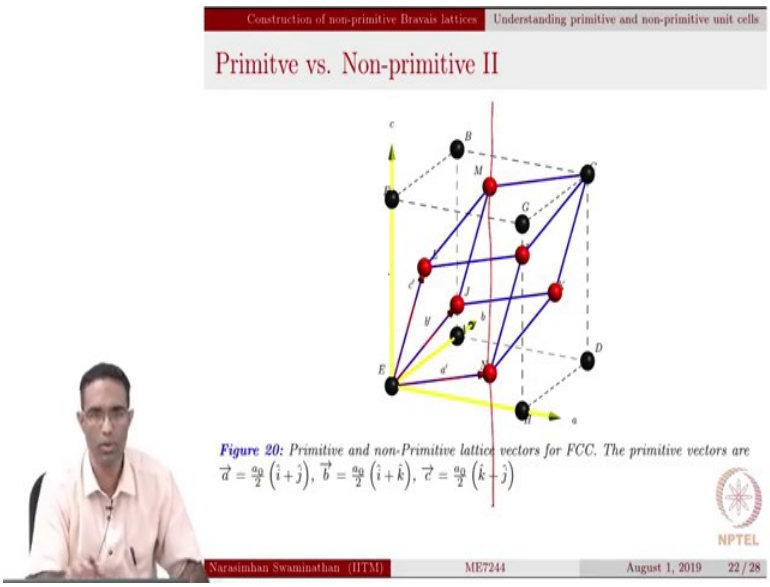

So for example, if we want to construct the FCC structure out of these lattice selectors, these are now non-primitive lattice vectors, We saw that when we had AIB sorry AJ and AK and if we wanted to construct the lattice vectors the total crystal structure turned out to be I mean the unit cells turned out to be non-primitive, you had more than one lattice point to the unit set.

However, if you want to use those non-primitive lattice vectors, we have to choose something called as basis. Basically there are four lattice points per unit cell in the non-primitive FCC structure. So we choose those four basis.

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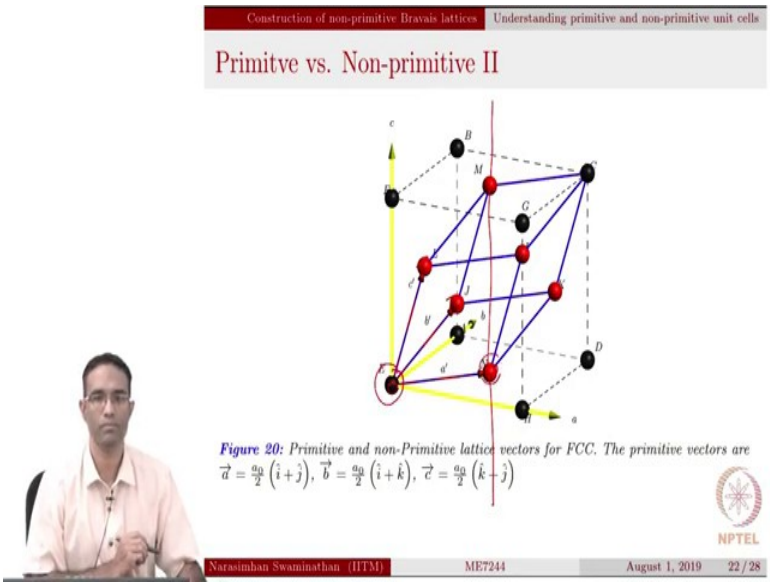

So these are the four basis. 1, 2, 3 and 4 The ones that are circled here. 1, 2, 3 and 4. And now, if you used these lattice vectors and constructed your crystal structure you would not be generating a FCC lattice So we just saw a simple MATLAB program for the simple cubic structure that was primitive. So there was no real, there was no line or anything that said anything about the basis for the crystal structure.

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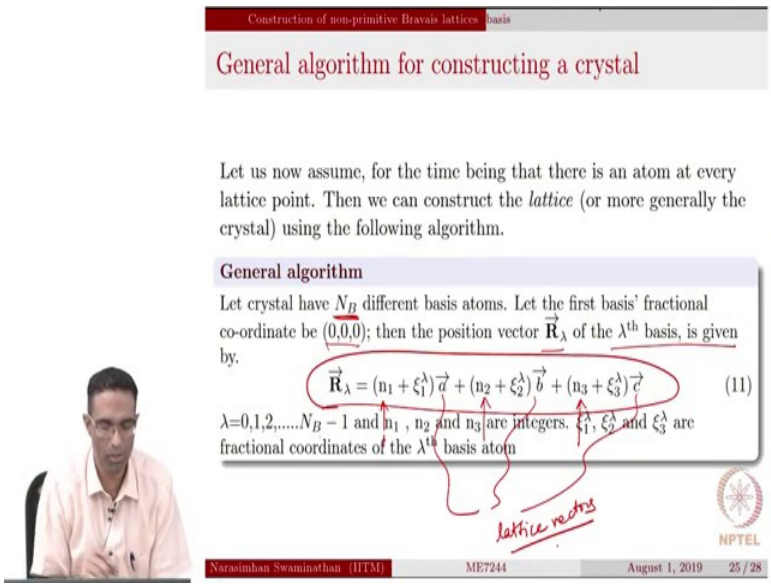

So now we will try to construct the FCC lattice and the general algorithm that is used in order to construct any crystal lattice is the following. So let us say that our crystal has NB different basis atoms. The basis atoms is the total number of atoms per unit cell system FCC, it was basically 4. Let the first basis fractional coordinate by 0 comma 000. That means you are putting your origin there.

Then a position r lambda, of the lambda basis is given by this expression right here. That is it. N1 is still the same set of integers and A, B and C are all the lattice vectors. C1 lambda, C2 lambda, C3 lambda are basically the first component of the fractional coordinate of the lambda to basis second component and the third component. And this can go from how many ever basis atoms you want. I put your lambda equals 0123 NB minus 1 because we have already counted 0, 0, 0 as one of the atoms right there.

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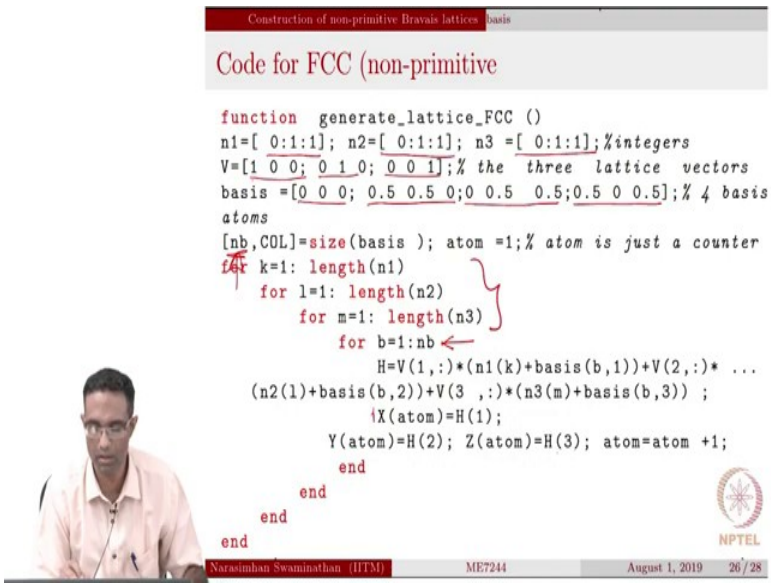

So this is basically the structure of the code that you will use if you want to generate a crystal structure out of non-primitive basis. So again you have N1 going from 0 to 1, 0 to 1, 0 to 1. So I am going to generate only one unit cell. V goes from 100, 010 and 001 which are basically the three lattice vectors. Now, the base is nothing but 000; 0.5, 0.5, 0; 0.5, 0.5; 0.5, 0, 0.5, the four values, the four atoms that I basically circled in the previous, in the picture that I showed you.

Now, in addition to the three loops that you have here, you have one additional loop that is going over all the basis, total number of basis atoms, so this will be four, NB is basically total number of basis atoms. And this formula here exactly replicates this expression right here. So h equal to the first vector times N1 which is basically an integer plus the basis, B2 times the second integer plus the basis b3 times the third integer plus the basis and the x coordinate will nothing but the h1, y coordinate is h2 and z coordinate will be h3, and there is a increment for the atom number.

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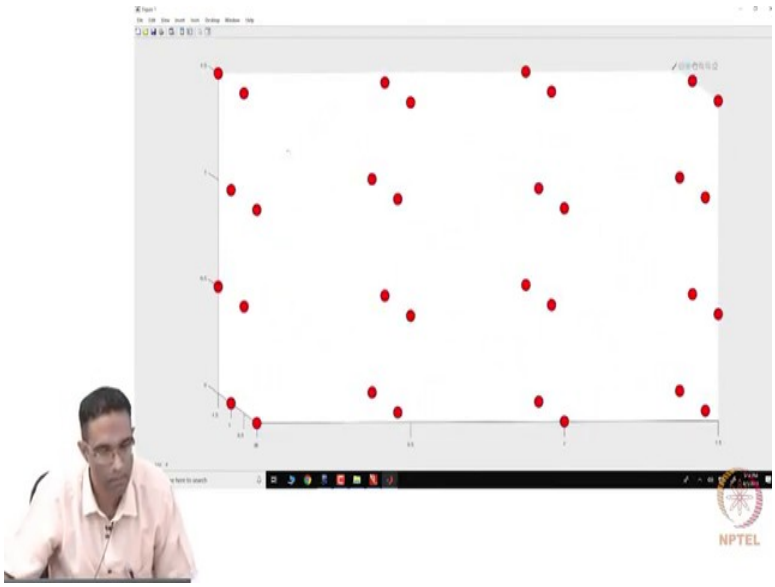

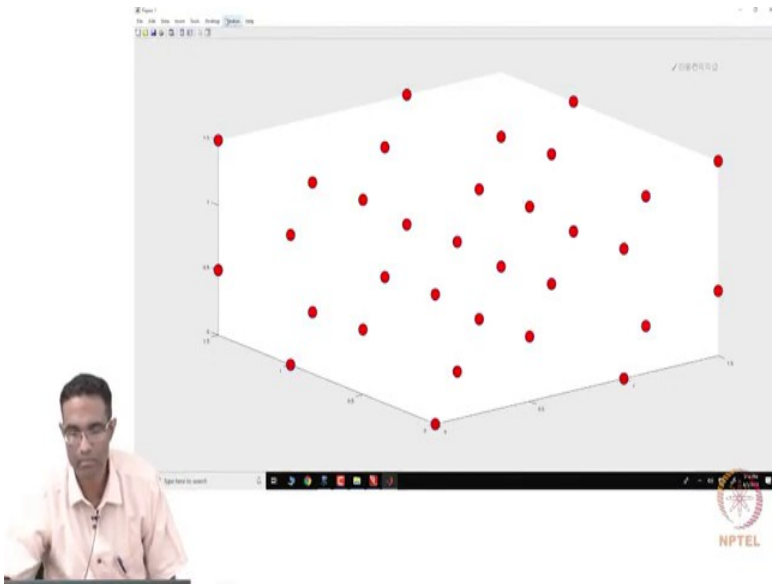

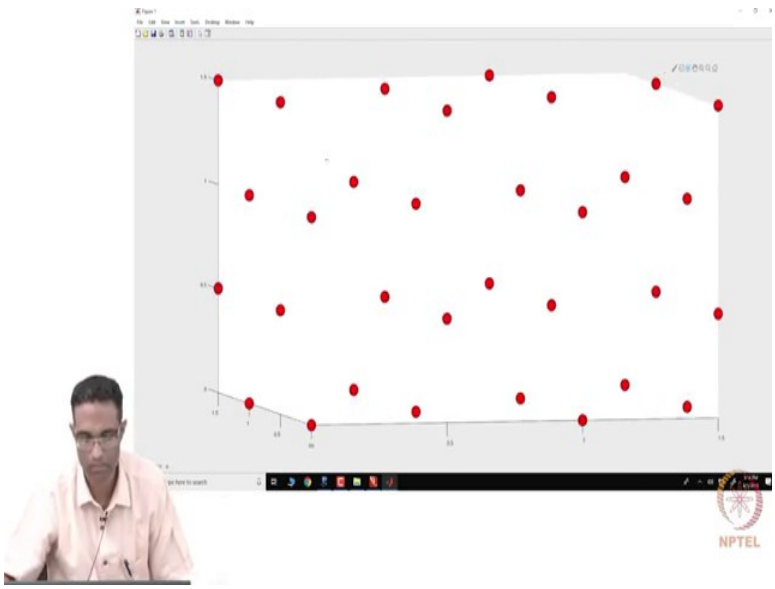

So once you run this code, you will actually be generating a, so I just ran that code right here. This is basically FCC structure. For example, if it is hard for you to notice, but look at this. And there is one atom right here. So one of the issues that we have here is that you find it hard to visualize one unit cell. So we will later on teach you how you can actually visualize just one unit cell using a MATLAB script. But otherwise, you know, it should be obvious to you that if you do not print certain atoms with certain coordinates which is greater than the lattice constant, then you will be able to visualize one unit cell of the FCC structure.

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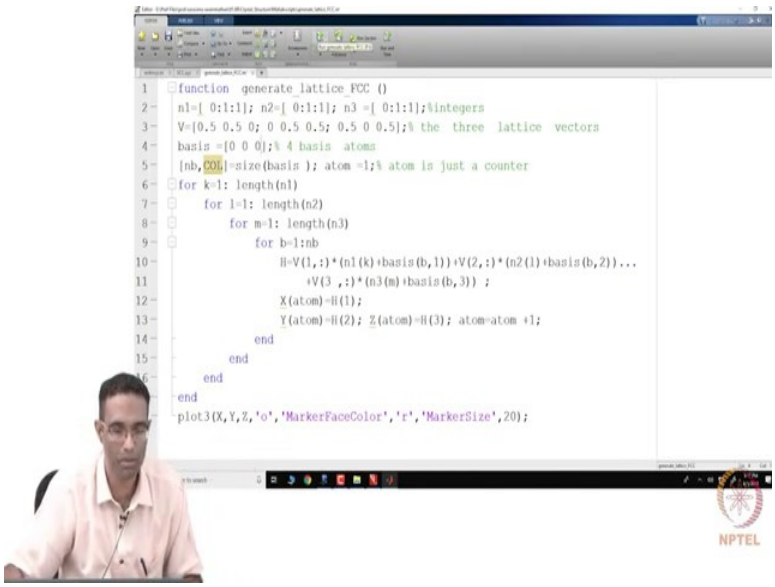

It is basically exactly the same code that I showed you in the PowerPoint slides, so you have the four basis atoms. nb basically consists of the total number of basis atoms and you have in addition to the previous loop n1, n2, n3 which we used for your primitive lattices, you have one more loop which goes over the total number of basis atoms. So are there any questions on this? Yes?

Student: Sir, can we change one lattice, FCC lattice assuming that non-primitive vectors ?

Professor: You can. You can print the FCC lattice using non-primitive vectors but I will demonstrate it probably later so that we can go ahead with this and we can do that little later. But it is possible.

All you have to do is if you want to generate with non-primitive lattice, what do you think you should do? That is a good question. The question is, how do we can we modify this code to generate our FCC structure with the primitive lattice? So what would you do? What were the lattice vectors for the primitive? A naught by 2 i plus j, So what I would do is, I would

change this to 0.5 0.5. Then I would change this to 0.5 0.5. And then the other combination 0.5 0.5.

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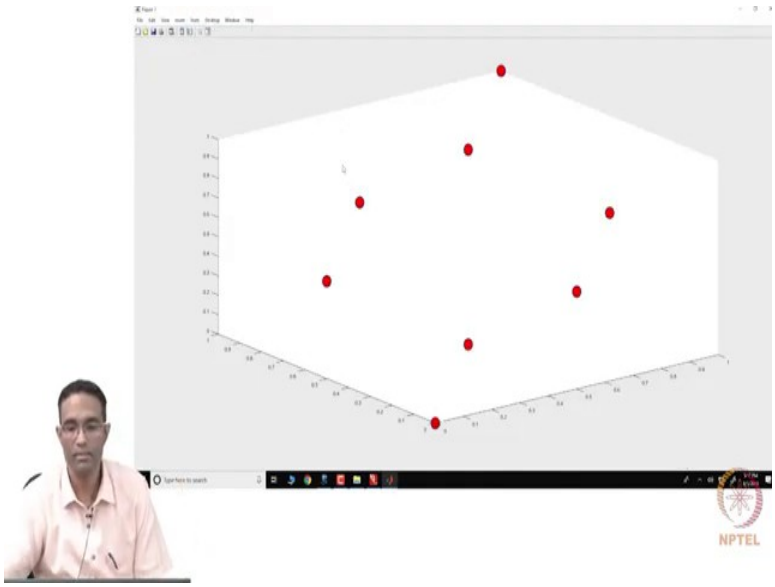

Now there is no basis, there is only one basis, which is my zero comma zero comma zero. But it will never look like your FCC lattices because these are the lattice vectors, This one is lying in the middle of the face of one cell, this one is lying in the middle of the face of the left hand side cell so it is going to be generating the lattice along those non orthogonal lattice vectors. So it will not look like FCC, but it has the symmetry of the cubic structure and it is in fact FCC

This is the way you modify your MATLAB codes to generate these non with the primitive or with the non-primitive. Generally we use non-primitive for FCC so that we want to retain the symmetry of the cubic structure.

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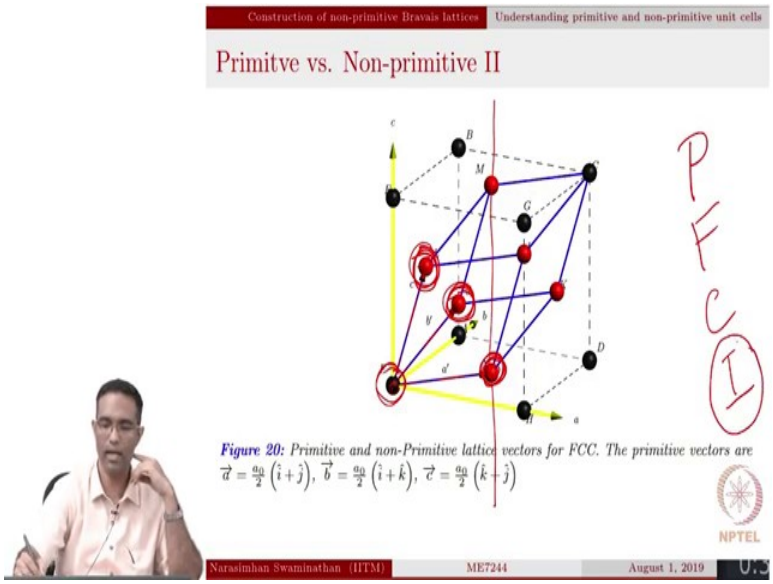

So you first asked the question how many lattice points are that per unit cell. So for FCC it is 4. So let us go back to this this diagram here. So this is one of the basis, zero comma zero comma zero will be one of the basis atoms. This will be the other basis, this will be the other basis and this will be other basis. If you choose this and this, they are equivalent, so these are the four basis atoms that you would choose for constructing your FCC structure using primitive lattice vectors.

But if you want sorry if you want using primitive lattice vectors, sorry non-primitive lattice vectors. For constructing non-primitive lattice vectors only you need 4 basis. For constructing primitive, if you want to use primitive lattice vectors then there is only one basis which is zero comma zero comma zero because it just contains one atom in the unit cell. Is this aspect clear? Do you have any questions on this? Primitive versus non-primitive becomes important

Whenever you see p, in this course whenever when we are talking symmetry you should understand that the lattice vectors that is associated with constructing this crystal structure is going to be primitive. When you see f, that means, the face entering lattice vectors has been used, which is basically it is no longer primitive, Similarly, for C and I.

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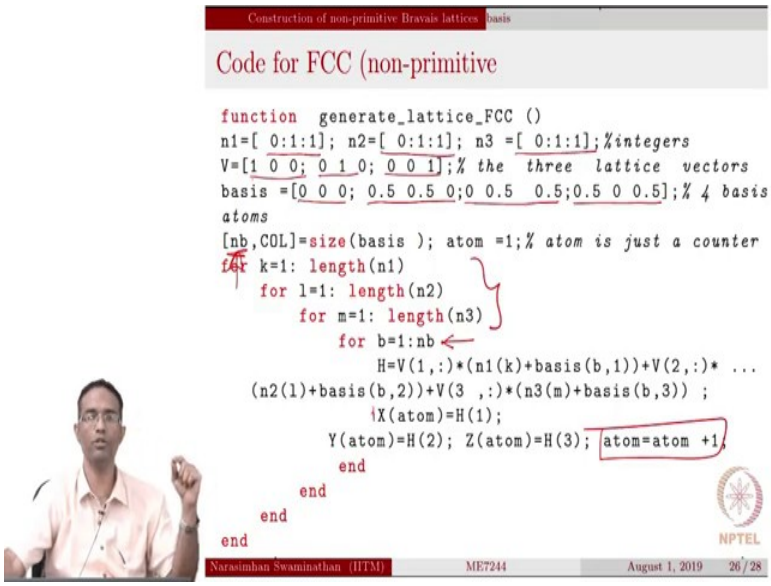

So you can in principle choose i. i will also have, so what would you do if you wanted to construct a body centered… suppose you wanted to modify this code to construct a body centered lattice how would you do it?

Student: two basis.

Professor: Hmm?

Student: (0,0.5,0)

Professor: Zero? No. The first one will be 000, the second one will be 0.5, 0.5, 0.5 and you can use a0i, a0j, a0k as your lattice vectors. It is also possible for you to choose primitive lattice vectors, but it is very hard to visualize that, but it is possible, I think that is one of the assignments that I have given you.

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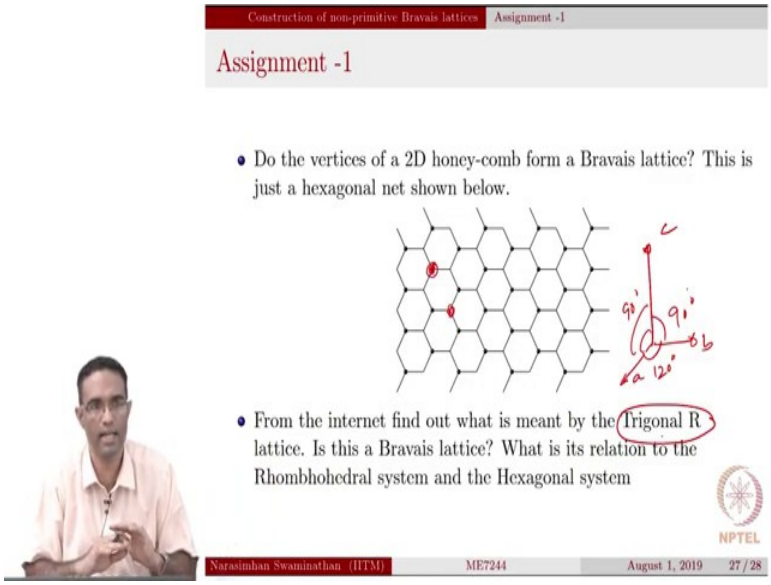

So one of the things that we discussed you know, previously, I just thought I will give you as an assignment, you can take a look at this hexagonal net. So this is just like how somebody mentioned the same environment is not seen by this lattice point and this latest point. Consequently an hexagonal net is not a Bravais lattice. You all have heard of trigonal lattice, R lattices, what is that?

Student: It is the rhombohedral one.

Professor: It is, what is that?

Student: All the lengths are different.

Professor: Two length will be same. So trigonal R has the same unit cell as the hexagonal So a, b, c and this included angle will be 120 degrees, and this and this is going to be 90 degrees It will look just like the hexagonal lattice, but there is something else that is going to be different about the tribunal which we will see when we study symmetry, The triagonal R,

rhombohedral and the triagonal R are basically the same crystal structures, They generate exactly the same lattice.

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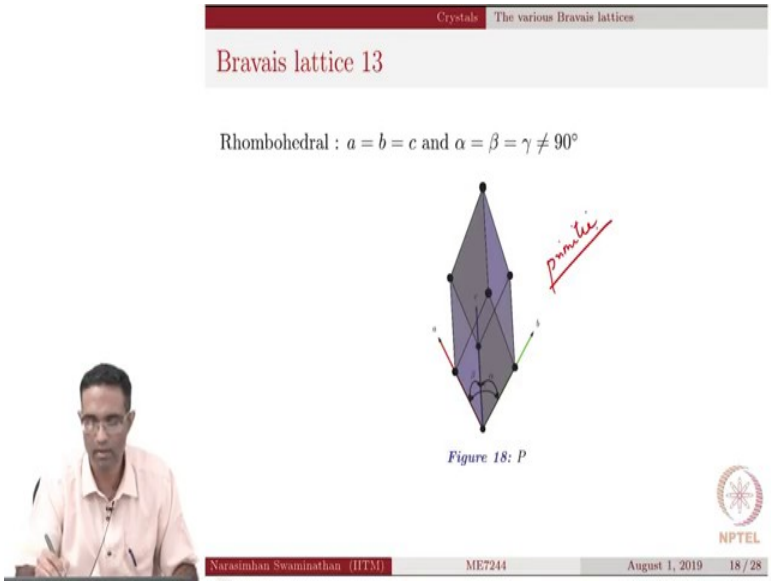

While trigonal R is non-primitive, the one that we saw here the rhombohedral is a equal to b equal to c, alpha equal to beta equal to gamma, but they are not 90 degrees is primitive,

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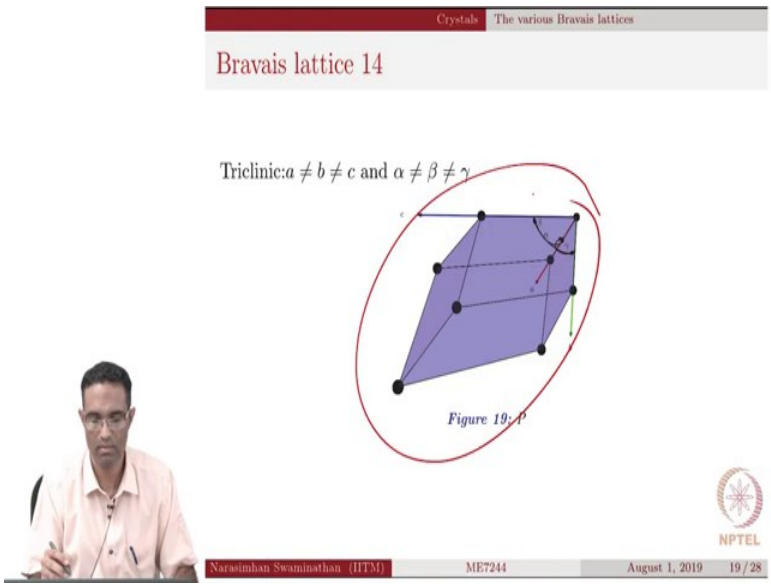

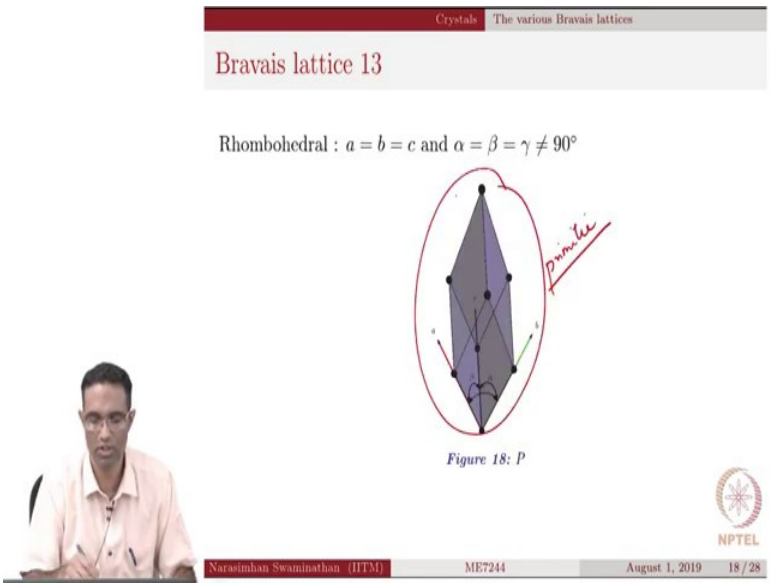

So off and on whenever we talk about rhombohedral and trigonal we generally use we can use the hexagonal unit cell in order to generate that lattice and inside that you can show that there is actually going to be this, the structure oh sorry, not this one, this one, this one, we can show that we will do that when we do symmetry in crystals.

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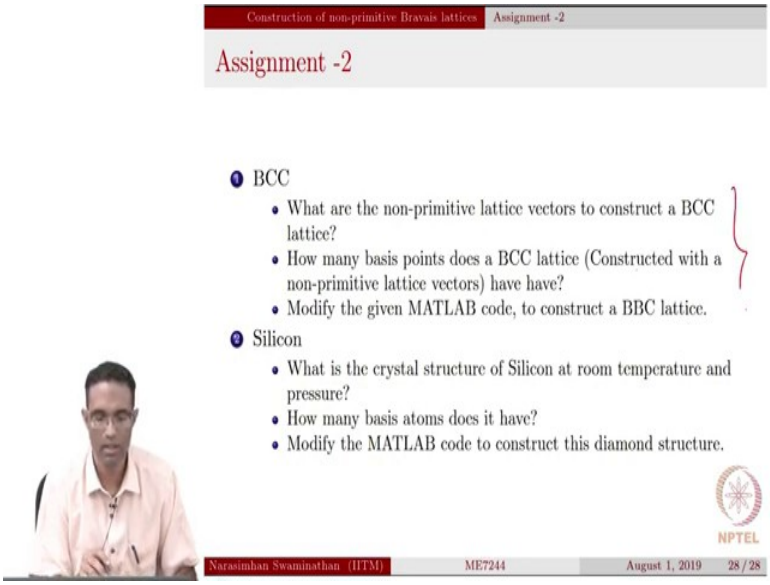

The next assignment that I want you to take a look at is what are the non-primitive lattice vectors to construct a BCC lattice. We just did that very quickly here. And I think I will share the codes with you and you should be able to modify this to generate these lattice structures and convince yourself that what you are getting is indeed a BCC. How many basis point, all that, this is the first assignment.

The second assignment is what is the crystal structure of silicon at room temperature and pressure, what is it?

Student: Diamond.

Professor: Diamond. So the question is how many basis atoms does it have and how will you modify this MATLAB code to actually construct your diamond structure? With regards to this Bravais lattices which is I know many of you might have already seen this in some format, do you have any other things or shall we just proceed with the next part of the lecture? We can proceed.

Student: Yes.

Professor: Okay.